

CHAPTER - 2

DEVELOPMENTS OF DIFFERENT THEORETICAL PREDICTIONS

The theoretical value of the differential cross section in which all the four elastic processes of scattering combine coherently is expressed in the general form by

$$\frac{d\sigma}{d\Omega} = \left| a^{(NT)} + a^{(R)} + a^{(D)} + a^{(NR)} \right|^2 \dots (2.1)$$

where the superscripts (NT), (R), (D) and (NR) refer to nuclear Thomson, Rayleigh, Delbruck and nuclear resonance scattering amplitudes respectively. Excepting nuclear Thomson scattering amplitude all other scattering amplitudes are complex e.g. $a^{(R)} = a_1^{(R)} + i a_2^{(R)}$ where the subscripts 1 and 2 refer to the real and imaginary parts respectively.

While using these amplitudes to calculate the differential cross sections, the photon polarization is taken into account. For linearly polarized photons, these amplitudes are expressed as components parallel (a_{11}) and

perpendicular (a_{\perp}) in the plane of scattering. The amplitudes for scattering of circularly polarized photons with no change of polarization are denoted by a_{NSF} and with change of polarization by a_{SF} . The scattering amplitudes for circularly polarized photons are related to the amplitudes for linear polarization by

$$a_{S.F.} = \frac{1}{2}(a_{\parallel} - a_{\perp}), \quad a_{NSF} = \frac{1}{2}(a_{\parallel} + a_{\perp}) \dots (2.2)$$

Since all the elastic scattering processes may act simultaneously they interfere with each other and it is necessary to know the relative phases of these scattering amplitudes in the sum (2.1). These relative phases have been reliably determined by Papatzacos²⁰.

2.1 Nuclear Thomson amplitudes

The nuclear Thomson scattering amplitude is well known for a given scattering angle θ and target atomic number Z . The amplitudes are expressed as components perpendicular and parallel to the plane of scattering in units of classical electron radius by

$$\cancel{a_{\perp}^{(NT)} = \frac{Z^2 m}{M}} \text{ and } \cancel{a_{\parallel}^{(NT)} = \frac{Z^2 m}{M} \cos \theta} \dots (2.1.1)$$

where m/M is the ratio of electron rest mass to the atomic mass and $m/h\nu = 1/1323 \lambda$ where λ is the atomic weight.

2.2 Rayleigh scattering amplitudes

The first attempt to calculate Rayleigh scattering amplitude was made by Franz²¹ in 1936 and was improved upon by Moon²² in 1950 and by Bethe²³ in 1952. His method widely known as the Form Factor Approximation is still being used with modifications. The differential elastic scattering cross section is given by

$$\cancel{\frac{d\sigma}{d\Omega} = \frac{r_0^2}{2} (1 + \cos \theta) |F(q, Z)|^2} \dots (2.3.1)$$

where $F(q, z)$ is the form factor for a given momentum transfer q , Z is the atomic number and r_0 is the classical electron radius. The form factor is expressed²⁴ as the matrix element

$$F(q, z) = \sum_{n=1}^Z \langle \psi_0 | \exp(iq \cdot r_n) | \psi_0 \rangle$$

... (2.2.2)

where ψ_0 is the ground state wave function of the atom, r_n is the radius vector from the nucleus to the n^{th} electron. The atomic form factor is also expressed²⁵ as

$$F(q, z) = \int \rho(r) \exp(iq \cdot r) d^3r$$

... (2.2.3)

where $\rho(r)$ is the total electron density at r . For a spherically symmetric atom the angular integrations are performed²⁶ resulting in

$$F(q, z) = 4\pi \int_0^{\infty} \rho(r) \frac{\sin qr}{qr} r^2 dr$$

... (2.2.4)

There have been many calculations and tabulations of atomic form factors, emphasis being given to the use of different wave functions. An excellent summary of these calculations is given by Hubbell⁹.

In his paper on form factor Franz²¹ proposed a correction to the form factor. Later, Brown and Mayers⁴ gave a semiempirical formula for correcting the form factor approximation. These are known as modified form factors. The modified form factor $g(q, z)$ is given by

$$g(q, z) = 4\pi \int_0^{\infty} \rho(r) \frac{\sin qr}{qr} \frac{1}{1 - E - V(r)} r^2 dr$$

... (2.2.5)

where $E = |\epsilon|$ is the energy of the electron and $V(r)$ is the atomic potential.

Tabulation of the non-relativistic atomic form factors (BMP) $F(q, Z)$ for $Z = 1$ to 100 and $q = .005\text{\AA}^{-1}$ to 10^3\AA^{-1} have been compiled by Hubbell⁹. These tables are constructed from the theoretical data of Brown^{27,28}, Cromer and Mann²⁹.

The recent addition is the tabulation of relativistic form factors (RFP) compiled by Hubbell¹⁰. It includes $F(q, Z)$ values for q from .01 to 10^3\AA^{-1} for elements $Z = 1$ to 100 from different researchers, viz., Boyle and Turner³⁰, Cromer and Weber³¹ and ~~Verob~~³².

A method for evaluating transition amplitudes for bound electrons in second order in the effect of the radiation field was outlined by G.E. Brown and his co-workers¹⁻⁴ in 1954-57. They described a method for solving the Dirac equation which describes the wave function including not only a small perturbing term but a large static potential. The effect of electron binding in the calculation of form factors were taken into account. During 1954-57 Brown and his co-workers published Rayleigh scattering amplitudes for photons scattered by K-shell electrons of mercury atoms at photon energies of 0.164,

0.327, 0.654 and 1.308 MeV using Coulomb potential. Later, Cornille and Chapdelaine³⁵ following Brown's procedure calculated Rayleigh scattering amplitudes for the K-shell electrons of mercury atoms for photon energy of 2.62 MeV.

It was almost a decade since Brown and his co-workers published results of Rayleigh amplitudes, Johnson et al^{34,35,6} extended Brown's procedure and published results of Rayleigh scattering amplitudes using D.H.F.S wave functions rather than the Coulomb wave functions as used by Brown. Johnson et al also extended their calculations to L and M shell electrons in certain cases. Johnson and Cheng⁵ have published results of Rayleigh scattering amplitudes at photon energies of 0.145, 0.279, 0.412, 0.662 and 0.839 MeV for lead atoms and at photon energies of 0.279 and 0.662 MeV for $Z = 30, 42, 56, 60$ and 73 .

The most recent and exhaustive calculations of Rayleigh scattering amplitudes from numerical solution of second order S-matrix have been done by Kissel and Pratt^{6,7}. They have used potential and wave functions resulting from DHS type self-consistent calculations. Kissel and Pratt have used Kohn-Sham exchange model rather than the Slater exchange model as used by Johnson and Cheng. Kissel and Pratt have reported^{6,7} Rayleigh

scattering amplitudes for the following atoms $Z = 2, 13, 30, 42, 47, 50, 62, 73, 74, 79, 80, 82$ and 92 for a wide range of photon energies starting from a few KeV upto 2.754 MeV for different inner shell electrons.

There is one more recent calculation of Rayleigh scattering amplitude made by Florescu and Gavrilă¹¹. They have evaluated matrix element for Rayleigh scattering amplitudes by K-shell electrons in the high energy limit and finite momentum transfer. The atomic field was assumed to be Coulomb in form. The integration in the momentum space was carried out by use of non-relativistic Green's function. They have published the results of scattering amplitudes H as a function of αZm where α is the fine structure constant. The Rayleigh amplitudes are given by

$$a_{\perp}^{(R)} = 2H \quad \text{and} \quad a_{\parallel}^{(R)} = 2H \cos \theta$$

... (2.2.6)

The values of H are available for $Z = 1, 6, 13, 29, 42, 50, 60, 73, 80, 82$ and 92 for values of $q/\alpha Zm$ from 0 to 15 .

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Table 1

Comparison of differential elastic cross sections (in unit of 10^{-26} cm²/sr) including Rayleigh and Thomson scattering amplitudes using Rayleigh amplitudes of Kiesel and Pratt and form factors.

ENERGY	ATOMIC NUMBER	q (°)	q in no	R.F. K L M	O.F.F. K L M	R.F. K L M N	O.F.F. K L M N	U.F.F. K L M N	E.O. (RHF) TOTAL AREA	
50.54 KeV	52	0.10	2.031	-04	5646.00	6235.63	27286.7	25599.7	27033.1	
		1.00	2.031	-03	5661.60	6229.00	27191.4	25504.99	27539.4	52702.6
		10.00	2.029	-02	5244.16	5799.62	19599.0	20604.87	19843.4	22562.6
		30.00	6.022	-02	2962.27	3372.62	3534.5	3970.17	3691.2	4181.87
		60.00	1.163	-01	653.85	830.86	693.16	866.19	766.8	867.61
		90.00	1.646	-01	186.41	263.92	224.19	306.23	258.9	315.63
		120.00	2.015	-01	130.28	199.87	144.82	214.38	173.6	218.89
		150.00	2.248	-01	136.37	223.30	142.38	223.16	169.6	230.89
		180.00	2.327	-01	142.29	239.65	145.16	241.33	182.4	244.32

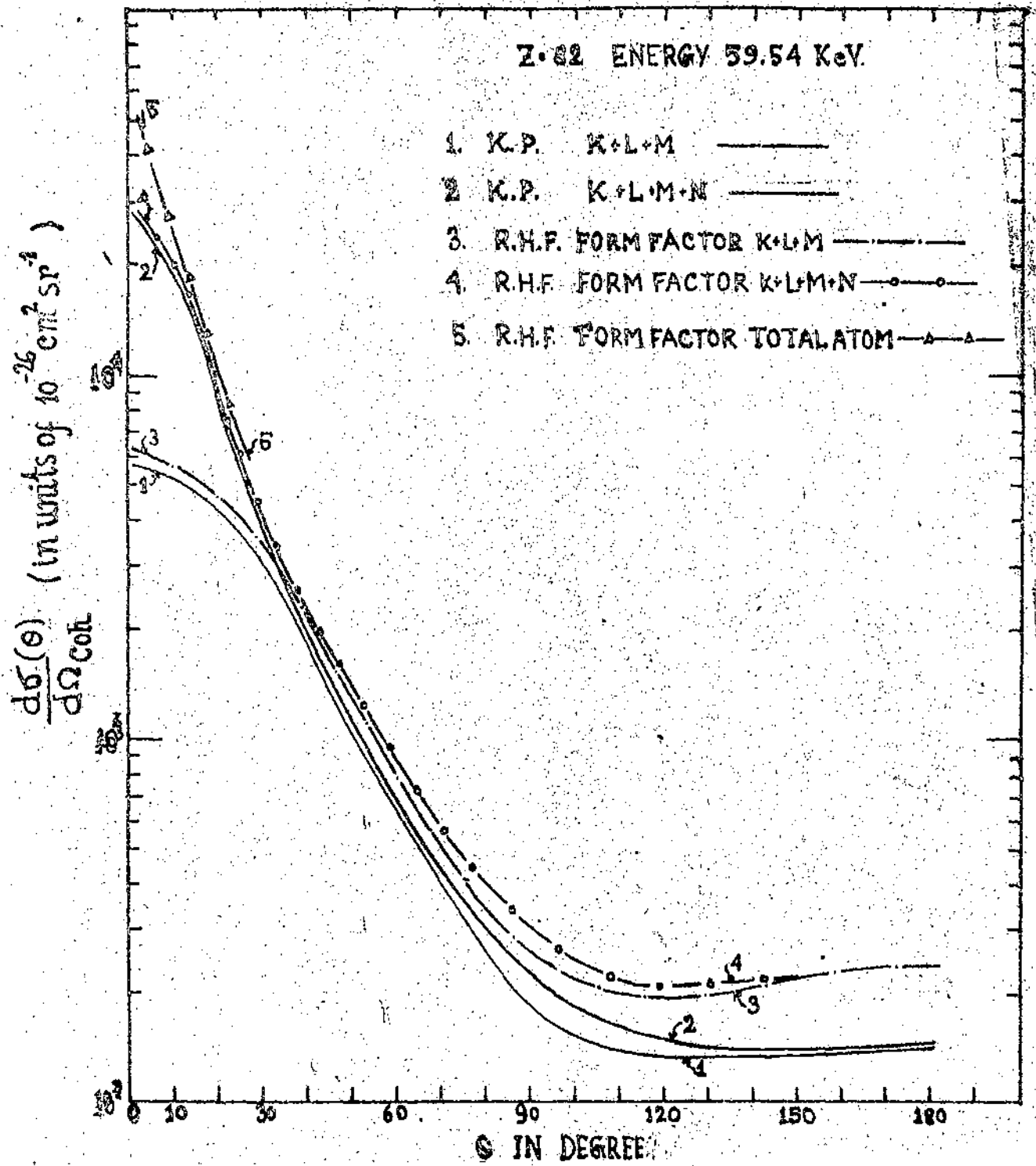


Fig. 1.

Table 2 Comparison of differential elastic cross section (in units of 10^{26} cm²/sr) including Rayleigh and Thomson amplitudes.

ENERGY KeV	ATOMIC NUMBER	$Q(^{\circ})$	q in m μ	K.P. R L M $\times 10^{-26}$	P.G. $\times 10^{-26}$	H.O(RHF) TOTAL ATOM $\times 10^{-26}$	J.O. R L M $\times 10^{-26}$	K.P. $\times 10^{-26}$	K.P. K real only $\times 10^{-26}$	RHF R L M $\times 10^{-26}$
145	82	1.00	4.964	-03	5949.10	47627.96		39.79	29.72	5859.61
		10.00	4.959	-02	4195.08	6399.05		38.92	29.13	4196.47
		30.00	1.472	-01	564.73	745.00	566.44	32.76	24.66	536.61
		60.00	2.345	-01	89.67	102.39	90.75	20.25	15.71	80.10
		90.00	4.023	-01	32.57	37.70	33.19	14.30	10.00	24.24
		120.00	4.930	-01	23.45	24.37	23.95	16.13	12.30	14.30
		150.00	5.493	-01	23.68	24.31	24.16	20.41	15.05	13.77

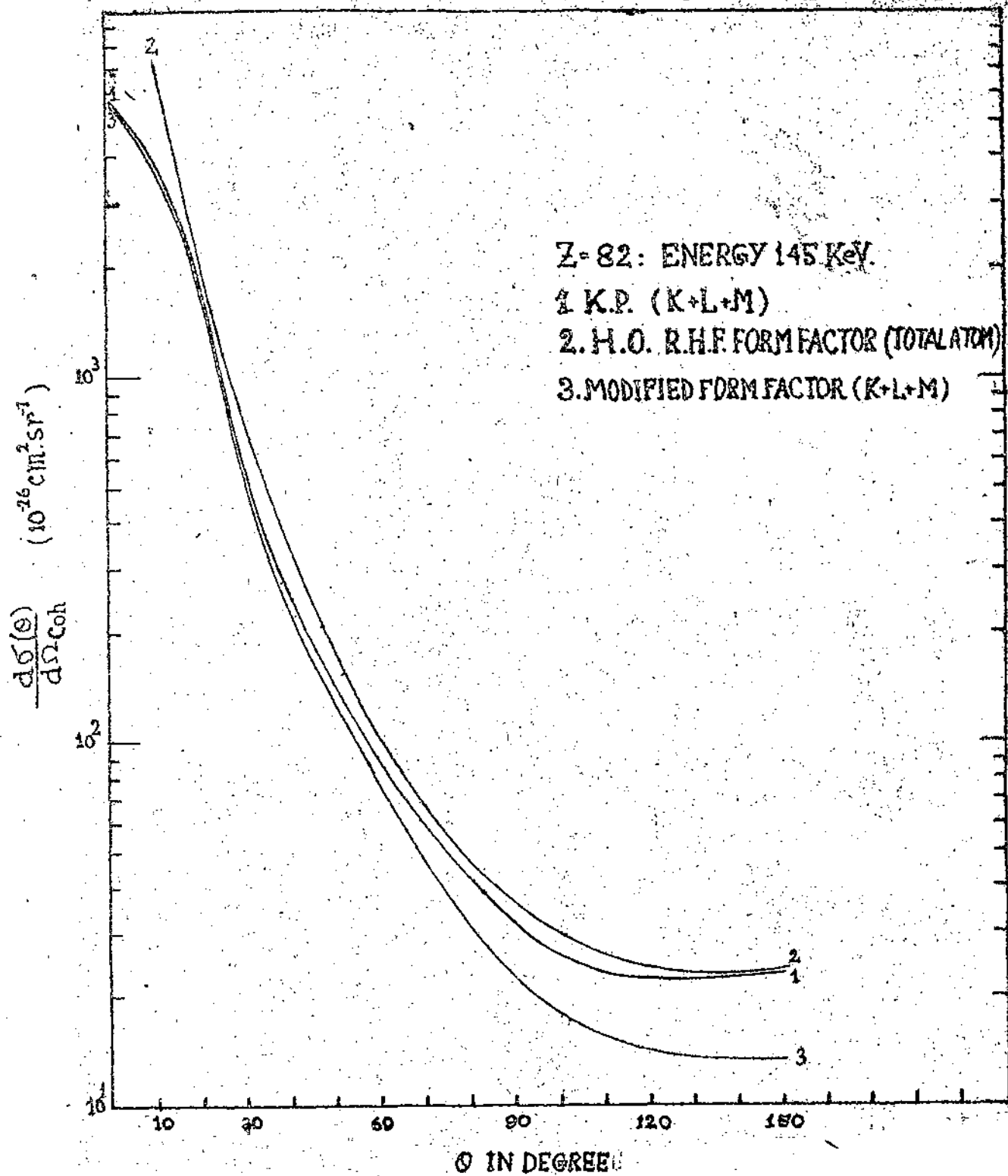


Fig. 2.

Table 3

Comparison of the sum of squared amplitudes (in units of classical electron radii)

ENERGY	ATOMIC NUMBER	$Q(\theta)$	g in hc	K.P. K L	J.G. K L	FORM FACTOR K L	MODIFIED FORM FACTOR K L	H.O. TOTAL ATOM FORM FACTOR	P.G. K	K.P. K
411.3 KeV	32	0.10	1.403 -03	90.29		99.99	88.21	6652.0	2.924	3.307
		1.00	1.406 -02	89.81		99.50	87.75	3901.9	2.916	3.304
		10.00	1.404 -01	54.93		62.38	53.53	117.8	1.867	3.076
		50.00	4.171 -01	5.963	4.000	5.630	3.831	7.375	1.650	1.734
		60.00	0.060 -01	0.4322	0.4334	0.6300	0.4379	0.6556	0.4367	0.4333
		90.00	1.139 00	0.1836	0.1844	0.5145	0.1404	0.3307	0.1171	0.1673
		120.00	1.595 00	0.1460	0.1468	0.2141	0.0808	0.2234	0.0602	0.1262
		150.00	1.558 00	0.1374	0.1382	0.2040	0.0679	0.2212	0.0474	0.1171
		180.00	1.611 00	0.1349		0.2047	0.0652	0.2231	0.0449	0.1146

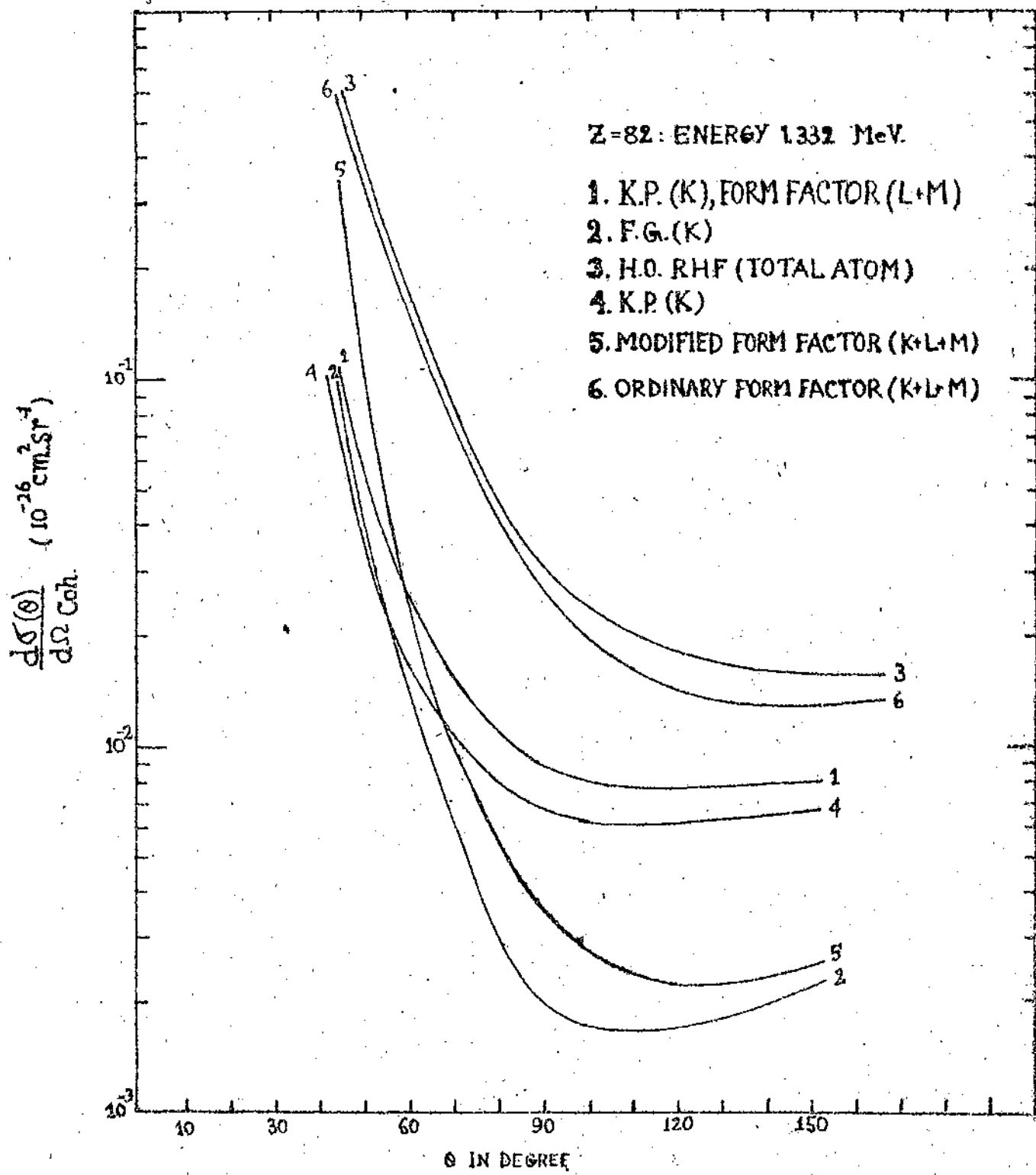


Fig. 3.

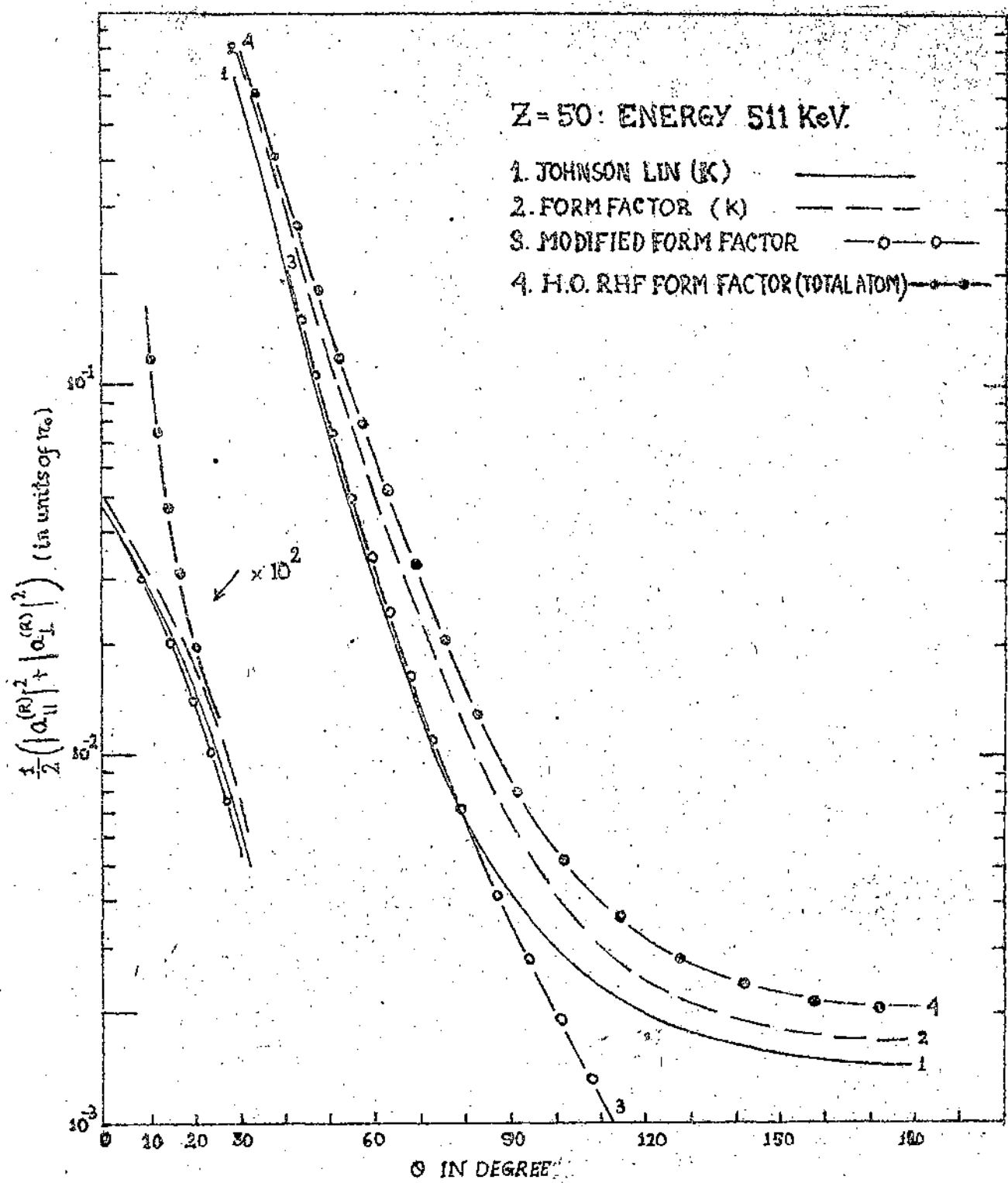


Table 5 Comparison of the sum of the squared Rayleigh scattering amplitudes (in classical electron radii) for K-shell electrons by Brown et al., Kissel and Pratt, Florescu and Gavrilă and total atom relativistic form factors due to Overbø and Hubbell are compared.

ENERGY	ATOMIC NUMBER	$Q(^{\circ})$	q in me	B.M. K-shell	K.P. K-shell	P.G. K-shell	H.O. (R.H.F.) TOTAL ATOM
1.303 MeV	80	0.00		2.889	3.098	2.9680	
		15.00	0.65 -01	0.9411		0.9695	1.733
		30.00	1.32 00	0.8600	0.0837	0.09622	0.8351
		45.00	1.96 00	0.006766		0.008244	0.08309
		60.00	2.56 00	0.00111	0.00121	0.007978	0.01617
		90.00	3.62 00	0.000699	0.000355	0.00000269	0.002197
		120.00	4.43 00	0.000483	0.000204		
		150.00	4.90 00	0.000477	0.000147		
		180.00	5.12 00	0.000430	0.000133		

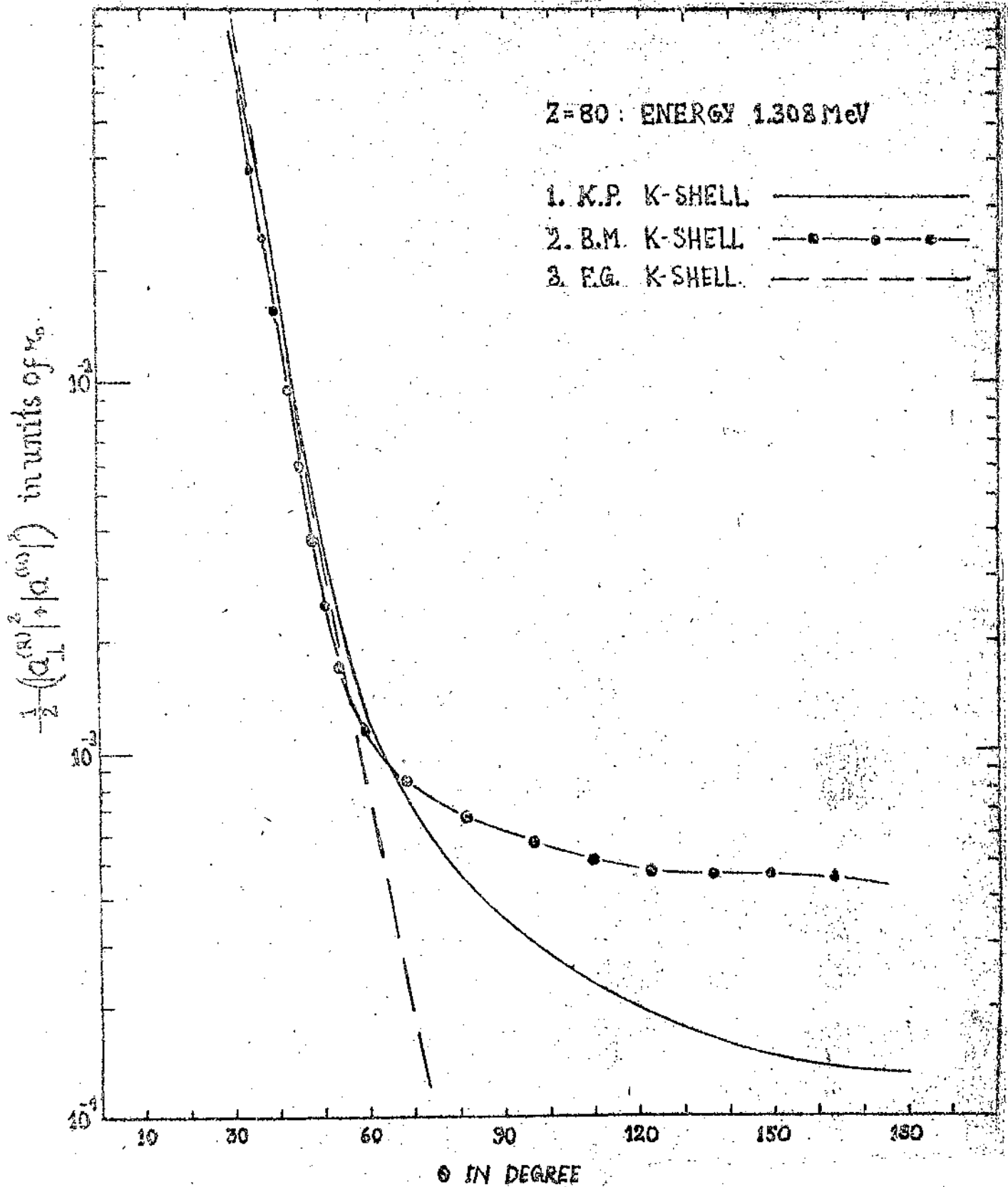


Fig. 5.

Table 6 Comparison of the sum of squared scattering amplitudes (in classical electron radii) electrons by Johnson & Lin, Floreanu & Savrills, Kessel & Pratt, K-shell modified form factor denoted by KMF, K-shell ordinary form factors denoted by KFF and total atom relativistic Hartree Fock form factors due to ~~Verha~~ and Hubbell.

ENERGY KeV	ATOMIC NUMBER	$q(^\circ)$	q in 10^3	J.L. K	F.O. E.	K.P. K	K.F.F.	K.M.F.	H.O.(RHF) TOTAL ATOM
511	50	0.00		3.606	3.535	3.014	3.9992	3.5373	
		10.00	1.74 -01	2.855	2.798		3.183	2.797	16.35
		20.00	3.46 -01	1.5065	1.485		1.738	1.468	1.906
		30.00	5.17 -01	0.6150	0.6115		0.7636	0.6082	0.7878
		40.00	6.84 -01	0.2245	0.2240		0.3654	0.2241	0.5527
		60.00	9.99 -01	0.03075	0.02948	.03071	0.05097	0.03139	0.06422
		90.00	1.41 00	0.004276	0.002478		0.006664	0.002314	0.003584
		120.00	1.73 00	0.002073	0.002042	.002073	0.002437	0.0007242	0.003248
		160.00	1.99 00	0.001415	0.001376	.001408	0.001668	0.0001782	0.002148

Table 7

Comparison of the sum of squared Rayleigh scattering amplitudes (in classical electron radii) for K-shell electrons by Johnson and Lin, Floreanu and Gavvilia, Kissel and Pratt and total atom R.H.P. form factors due to ~~verb~~ and Hubbell and non-relativistic form factors due to Greiner et al are compared.

ENERGY KeV	ATOMIC NUMBER	$\theta(^{\circ})$	g in mc	F.C. K	J.L. K	R.P. K	O.H. (RHP) TOTAL ATOM	GREIER (RHP) TOTAL ATOM
40.99	13	0.00		3.964	4.0442	4.0435		
		30.00	4.14 -02	2.818	2.9384		7.611	7.566
		60.00	7.99 -02	1.283	1.3158	1.5150	1.186	1.2169
		92.00	1.13 -01	0.5871	0.6989		0.5514	0.5497
		120.00	1.33 -01	0.4281	0.4654	0.4654	0.4583	0.4471
		150.00	1.54 -01	0.4525	0.4712		0.4513	0.4607
		180.00	1.59 -01	0.4618	0.4814	0.4814	0.4610	0.4633

Table 3

Comparison of the sum of squared Rayleigh scattering amplitudes (in classical electron radii) for K-shell electrons by Kissel and Pratt, Florescu and Gavrilu and total atom form factors by Hubbell and ~~Averb~~ are compared.

ENERGY KeV	ATOMIC NUMBER	q in m μ	F.C. K-shell	H.C. (R.H.F) TOTAL ATOM	K.P. K-shell
145.4	13	0.00			5.974 00
		5.00	2.43 -02	3.653 00	3.672 00
		10.00	4.96 -02	3.072 00	2.924 00
		20.00	9.93 -02	1.436 00	1.320 00
		30.00	1.47 -01	3.312 -01	4.656 -01
		45.00	2.17 -01	1.044 -01	6.753 -02
		60.00	2.84 -01	2.230 -02	1.863 -02
		90.00	4.01 -01	2.228 -03	1.653 -03
		120.00	4.92 -01	6.770 -04	6.164 -04
		150.00	5.49 -01	4.230 -04	4.068 -04

Table 2 Comparison of the sum of squared Rayleigh amplitudes (in classical electron radii) for K-shell electron by Kinsell and Pratt, Floresca and Gavrilla and total atom relativistic form factors by Hubbell and ~~Verby~~ are compared.

ENERGY	ATOMIC	$\theta(^{\circ})$	q in m μ	P.G. K-shell	H.G. (R.H.E) TOTAL ATOM	K.P. K-Shell
279.2 KeV	13	0.00				3.957 00
		5.00	4.765 -02	3.027 00	5.727 00	3.018 00
		10.00	9.520 -02	1.590 00	1.449 00	1.473 00
		20.00	1.897 -01	2.323 -01	2.358 -01	2.004 -01
		30.00	2.823 -01	3.104 -02	3.317 -02	2.690 -02
		45.00	4.131 -01	2.499 -03	2.775 -03	2.053 -03
		60.00	5.459 -01	3.132 -04	3.639 -04	2.536 -04
		90.00	7.725 -01	1.715 -05	2.309 -05	1.702 -05
		120.00	9.462 -01	3.713 -06	6.434 -06	5.144 -06
		150.00	1.055 00	2.439 -06	3.841 -06	3.236 -06

Comparisons of different calculations of Rayleigh scattering amplitudes available in literature are made with the help of some tables 1-9 and plots (Figs. 1-5), covering low, medium and high Z atoms as a function of energy and scattering angles.

2.5 Delbruck scattering amplitudes

The first theoretical work on Delbruck scattering was done by Kemmer³⁶ in 1937 and was restricted to photon energies $w \ll m$. At the same time in 1937 Akhiezer and Pomerenchuk³⁷ worked on high energy cases. They pointed out that the Delbruck amplitudes are proportional to e^4 though immediately after the Delbruck effect was proposed Oppenheimer³⁸ suggested that the transition probability of Delbruck scattering was of the order of $(\alpha Z)^4$. Akhiezer and Pomerenchuk³⁷ obtained same type of expressions as Kemmer's and obtained results for $m \ll q \ll w$. Akhiezer, Pomerenchuk and Kemmer missed the imaginary part of Delbruck amplitudes which dominates at high photon energies. The later calculations of Delbruck amplitudes were approached by two different ways. It was related either to pair production or to vacuum polarization. Jost et al.³⁹ showed the relationship between Delbruck scattering and pair production from the unitarity of S -matrix and calculated

Delbruck amplitudes restricted to imaginary parts and to the forward direction only.

Rohrlich and Gluckstern⁴⁰ used dispersion relation to obtain real part of the Delbruck amplitudes with the help of the value of σ_{pp} calculated by Jost et al³⁹. They checked the formulae so obtained with direct calculation of real and imaginary parts of Delbruck amplitudes from the diagonal S-matrix element. They used the Dyson-Dyson formulation of quantum electrodynamics for the first time in calculating these amplitudes.

At the same time Bethe and Rohrlich⁴¹ calculated Delbruck amplitudes in the high energy limit starting from optical theorem and ignoring photon polarization in the process.

An important work was done by Kessler⁴² in 1958, generalising a method for computing non-diagonal matrix elements of S^4 from S^2 . He obtained imaginary parts of the amplitudes parallel and perpendicular to the plane of scattering for arbitrary values of scattering angles as a five fold integrals. Integrations were performed for photon energy of 2.64 MeV and at scattering angle 90° . Sernik⁴³ extended Kessler's calculation to photon energy of 6.14 MeV upto scattering angle 180° . Endtaky and Shepp¹³ used the formula derived by Kessler to

calculate the imaginary parts of the amplitude for a wide range of photon energies from 1 to 20 MeV and scattering angles upto 120° . They obtained real parts in the form of six fold integrals with the help of fixed angle dispersion relation.

Recently Papatzacos and Nork¹² have calculated Delbruck amplitudes for a wide range of photon energies w varying from $w \leq 1$ MeV to several GeV from fourth order vacuum polarization tensor using Feynman technique in the lowest order Born approximation. Gauge invariance was applied to write the amplitudes. The integrals were reduced to four fold integrals by analytic integrations. The other integrals were calculated numerically. They have published results which differ from those obtained by Kholtzky and Shepp¹³ in real part of the amplitudes.

Between the work of Kholtzky and Shepp on the one hand and that of Papatzacos and Nork on the other, Constantini et al⁴⁴ derived formulae for Delbruck amplitude in the form of three fold integrals, the integrands containing many dilogarithm functions for the real part of the amplitudes. In 1978 Dr. De. Tollis et al⁴⁵ manipulated the formulae obtained earlier and simple expressions were obtained in the form of a sum of two fold and three fold integrals containing rational, irrational and logarithm

functions. They have published results at 10.83 MeV photon energy and scattering angles from 50° - 150° . Their results agree with Papatzacos and Mork's result on the real part of the amplitudes compared to those obtained by Ehlitzky and Shepp. In 1976 Barnoy and Rahane⁴⁸ calculated imaginary parts of Delbruck amplitudes following the work of Constantini for photon energies ranging from 1.33 MeV to 28 MeV and for scattering angles from 0° to 180° .